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First-principles study on scattering potentials of defects on Ge(001) surfaces TOMOYA ONO, Osaka University — As new techniques for the nanoscale manipulation and modification of materials progress, the electron scattering properties of nanostructures are the focus of attention both experimentally and theoretically. The spatial maps of the local density of states obtained by scanning tunneling spectroscopy can give us the images of standing waves, which provide important information about the dispersion relation of the electron scattering process at the potential barrier. I examined the scattering potential of the Ge-Si and Ge-Sn dimers on Ge(001) surfaces using a first-principles calculation. By calculating the scattering wave functions, the standing waves in the spatial map of the local density of states are examined; the waves correspond to the image of the differential conductance obtained by scanning tunneling spectroscopy. The period of the standing wave and its phase shift agree with those obtained by the experiment. I found that the scattering potential acts as a barrier when the electronegativity of the upper atom of the dimer is larger than that of the lower atom, while it becomes a well in the opposite case. The scattering potential is related to the stabilization of the ? bands of the Ge(001) surface due to the difference in electronegativity between Ge and the impurity.

Tomoya Ono
Osaka University

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